

An efficient prescription to find the eigenfunctions of point interactions Hamiltonians

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Abstract

A prescription invented a long time ago by Case and Danilov is used to get the wave function of point interactions in two and three dimensions.

1 Introduction

Consider the free particle s -wave time-independent Schrödinger equation in $D = 2$ and $D = 3$ dimensions. The radial part of the Schrödinger equation is given by

$$-\frac{\hbar^2}{2m} \frac{1}{r^{D-1}} \frac{d}{dr} r^{D-1} \frac{d\psi_k(r)}{dr} = E\psi_k(r) \quad (1)$$

The most general solutions are given by

$$\psi_k(r) = \cos(\eta(k)) J_0(kr) - \sin(\eta(k)) N_0(kr) \quad (2)$$

for $D = 2$ dimensions and

$$\psi_k(r) = \cos(\eta(k)) \frac{\sin(kr)}{r} - \sin(\eta(k)) \frac{\cos(kr)}{r} \quad (3)$$

for $D = 3$ dimensions. In equations (2) and (3), $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $J_0(kr)$ and $N_0(kr)$ in equation (2) are the Bessel and Neumann functions [1], respectively.

One usually disregards the irregular solution on the grounds that it goes to infinity at the origin. However, although the wave function diverges, the probability of finding the particle in a small region around the origin is finite and so, in fact, there is no reason to reject the irregular solution.

The question to be answered is if there exists self-adjoint operators (Hamiltonians), such that (2) and/or (3) are eigenfunctions of such operators. It can be proved [2, 3] that for both cases (eigenfunctions (2) and (3)) there exists a family of operators depending on one parameter that have functions of this form as eigenfunctions. The eigenfunctions of such operators are given by (2) and (3) with an appropriate choice of the functions $\eta(k)$ which as we shall see depend on one parameter that can be taken as, or is related to, the strength of the interaction. Since the eigenfunctions are indistinguishable from the free particle eigenfunctions for $r > 0$ one usually says that these Hamiltonians correspond to the free Hamiltonian plus a point interaction at the origin. Other common name for these interactions are contact interactions, zero-range interactions or Fermi pseudo potentials.

The subject can be approached from a number of different points of view. First one can use the theory of self-adjoint extensions [2, 3, 4]. This approach demands a certain mathematical maturity and although is by far the most complete approach it can hardly be considered pedagogical for undergraduate students.

Another approach is to use a finite range potential and take the zero range limit of the potential allowing its strength to diverge suitably. This regularization procedure has been used for instance in references [5, 6, 7, 8]. This process is simple but can be very laborious.

A third approach is to add Dirac delta function like distributions to the free Hamiltonian. This approach is considered, for example, in the papers Kurasov [9, 10] and again is a little advanced to undergraduate students.

Some time ago a prescription to handle point interactions was invented by Danilov [11] in the context of many body problems and in a slightly different context by Case [12]. This prescription was rediscovered [13] in the context of the scattering of particles by an Aharonov-Bohm potential.

The purpose of this note is to present Case-Danilov's prescription in the context of a free particle interacting only with a "point interaction" in $D = 2$ and $D = 3$ dimension where it can be learned easily.

Interest in quantum mechanics problems involving point interactions is continuing since it was introduced by Fermi [14]. A few recent examples of the its use can be found in the following references [15, 16, 17, 18, 19, 20] and in the references therein. The fact that point interactions is so popular is due to the fact that these problems are frequently solvable [2].

2 The Case-Danilov prescription

Case-Danilov's prescription teaches us how to find $\eta(k)$. It consists in imposing that two eigenfunctions of different energies be orthogonal, that is

$$\int_0^\infty \psi_k^*(r)\psi_\ell(r)r^{D-1}dr \propto \delta(k - \ell) \quad (4)$$

For a general $\sin(\eta(k))$ and $\cos(\eta(k))$, the right hand integral contains terms which are not proportional to $\delta(k - \ell)$. By choosing $\eta(k)$ in such way that those terms cancel, we get the wave functions of the self-adjoint family of operators. One should note that certain integrals that appear below are improper in the ordinary sense and should be evaluated according, for example, the prescriptions given by Brownstein [21].

This prescription was applied by Case [12] to find the eigenfunctions of a particle moving under the influence of a potential of the form $\frac{1}{r^2}$. The Case-Danilov prescription can be applied to find point interactions every time one finds that the time independent Schrödinger equation has two linear independent solutions that are square integrable. We mention a few examples at the end of this note.

3 Calculations

Consider first the two dimensional case. Using the indefinite integral [1]

$$\begin{aligned} & \int^Z \left[(k^2 - \ell^2)t - \frac{(\mu^2 - \nu^2)}{t} \right] J_\mu(kt) N_\nu(\ell t) dt = \\ & = Z[kJ_{\mu+1}(kZ)N_\nu(\ell Z) - \ell J_\mu(kZ)N_{\nu+1}(\ell Z)] - (\mu - \nu)J_\mu(kZ)N_\nu(kZ) \end{aligned} \quad (5)$$

and using the asymptotic forms when $Z \rightarrow 0$ or $Z \rightarrow \infty$ of the Bessel function ([1], p. 360 for small Z and p. 364 for large Z), we get (see reference [13] for

more details and other cases)

$$\begin{aligned} \int_0^\infty \psi_k^*(r)\psi_\ell(r)rdr &= \frac{2}{\pi} \tan(\eta(k)) - \frac{2}{\pi} \tan(\eta(\ell)) + \\ &+ \frac{4}{\pi^2} \tan((\eta(k)) \tan(\eta(\ell)) \ln\left(\frac{k}{\ell}\right) + \frac{1}{\sqrt{k\ell}} \delta(\ell - k) \end{aligned} \quad (6)$$

where the terms not proportional to $\delta(k - \ell)$ come from the lower limit of integration. These terms have to cancel out and this occurs if we impose

$$\tan(\eta(k)) = \frac{\pi}{2} \frac{-1}{\ln(k_b/k)} \quad (7)$$

The physical meaning of the parameter k_b , which we note is positive, will be explained below.

Consider now the three dimensional case. Again integrating we find that

$$\int_0^\infty \psi_k^*(r)\psi_\ell(r)r^2dr = \frac{1}{\ell^2 - k^2} [-\tan(\eta(k))\ell + \tan(\eta(\ell))k] + \frac{\pi}{2} \delta(k - \ell) \quad (8)$$

where once again the terms not proportional to $\delta(k - \ell)$ come from the lower limit of integration. In order to cancel these terms, we impose

$$\tan(\eta(k)) = -\frac{k}{k'_b} \quad (9)$$

where k'_b can be positive or negative. This equation can also be derived from equation (A3) on p. 175 of reference [21].

The physical meanings of the parameters k_b in equation (7) and k'_b in equation (9) are as follows. Comparing equation (7) with equation (18) of reference [5], we see that k_b is linked with the arbitrary energy of a unique bound state through $k_b = \sqrt{\frac{2m}{\hbar^2} E_b}$. The interpretation of k'_b is obtained by observing that $k \cot(\eta(k)) = -k'_b$ so that k'_b is the inverse of the scattering length. Since k'_b can be positive or negative, the system may or may not possess a bound state.

As other examples of cases where the Case-Danilov prescription can be applied, the reader can try it for the s -wave function of the hydrogen atom [22], for the s -wave harmonic oscillator [20] in one, two and three dimensions or for the one-dimensional hydrogen atom [23].

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